Development of Hierarchical Multiscale Method and Its Applications to the Characterization of Microstructure Effect

I-Ling Chang, Associate Professor
Department of Mechanical Engineering,
National Chung Cheng University,
Ming-Hsiung, Chia-Yi 621,
TAIWAN

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
08 FEB 2011	**FInal**	**10-06-2009 to 10-06-2010**

4. TITLE AND SUBTITLE
Development of Hierarchical Multiscale Method and Its Applications to the Characterization of Microstructure effect

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
I-Ling Chang

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
National Chung Cheng University,168 University Rd., ,Min-Hsiung,Chia-Yi Taiwan,TW,621

8. PERFORMING ORGANIZATION REPORT NUMBER
N/A

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AOARD, UNIT 45002, APO, AP, 96337-5002

10. SPONSOR/MONITOR'S ACRONYM(S)
AOARD

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AOARD-094152

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The mechanical properties of materials are inherently multiscale, depending on phenomena at all length scales. Hence, multiscale modeling is a huge scientific challenge as well as a critical necessity for successful manipulation of material properties. This proposed research aims to investigate the microstructure (i.e., grain and inclusion) effect on the material properties especially for the system which involve two characteristic microstructure features at distinct length scales using hierarchical multiscale method. The fundamental understanding of multiscale behavior is the key to the utilization of nano-materials and to the design of material systems contained nano-materials. In polycrystalline nanofilm, two distinct characteristic sizes, i.e. grain size of micrometers and film thickness of nanometers, are involved. The typical size of inclusion would vary significantly due to manufacturing process. The hierarchical multiscale simulation method, which integrates atomistic and continuum methods sequentially, offer the possibility to characterize the size dependence of both elastic and plastic properties. The proposed innovative algorithm adopts the representative volume element concept to link atomistic and continuum models through the parameters of the finite element method, which permits a reduction of the full set of atomistic degrees of freedom. This research gives a description of the proposed innovative method with special reference to the ways in which the method may be used to model crystals with more than a single grain or inclusion. In the project, we utilized the proposed innovative multiscale method to study the microstructure effect on the material properties. A multiscale method is developed to bridge the gap between nano-scale and macro-scale and study the multiscale behavior of materials. Ultimately, we developed a systematic approach to gain physical insight of the multiscale behavior of nano-materials for the design and fabrication of nano-devices.

15. SUBJECT TERMS **Modelling & Simulation, multiscale**					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**Same as Report (SAR)**	**23**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

Abstract

The mechanical properties of materials are inherently multiscale, depending on phenomena at all length scales. Hence, multiscale modeling is a huge scientific challenge as well as a critical necessity for successful manipulation of material properties. This proposed research aims to investigate the microstructure (i.e., grain and inclusion) effect on the material properties especially for the system which involve two characteristic microstructure features at distinct length scales using hierarchical multiscale method. The fundamental understanding of multiscale behavior is the key to the utilization of nano-materials and to the design of material systems contained nano-materials.

In polycrystalline nanofilm, two distinct characteristic sizes, i.e. grain size of micrometers and film thickness of nanometers, are involved. The typical size of inclusion would vary significantly due to manufacturing process. The hierarchical multiscale simulation method, which integrates atomistic and continuum methods sequentially, offer the possibility to characterize the size dependence of both elastic and plastic properties. The proposed innovative algorithm adopts the representative volume element concept to link atomistic and continuum models through the parameters of the finite element method, which permits a reduction of the full set of atomistic degrees of freedom. This research gives a description of the proposed innovative method with special reference to the ways in which the method may be used to model crystals with more than a single grain or inclusion.

In the project, we utilized the proposed innovative multiscale method to study the microstructure effect on the material properties. A multiscale method is developed to bridge the gap between nano-scale and macro-scale and study the multiscale

behavior of materials. Ultimately, we developed a systematic approach to gain physical insight of the multiscale behavior of nano-materials for the design and fabrication of nano-devices.

Introduction

The recent development of nanotechnology opens unique opportunities to explore the underlying mechanisms that affect the material behaviors embedded behind the continuum homogenization approach. The material behaviors are collective results of different mechanisms interconnect and interact at several length scales. For example, microstructural features in metals, e.g., impurities, dislocations, grain boundaries, profoundly affect what happens on a larger scale, particularly when systems are pushed to their limits. In order to comprehensively understand or even manipulate the material properties, the multiscale analysis method that can deal with the mechanisms at different scale is essential. To meet this demand, the proposed research developed a multiscale approach that hierarchically combines the models of different scales so that an accurate and efficient computation scheme could be realized. The proposed approach will then be used for the investigation of the microstructure effect on the material properties especially for the system which involve two characteristic microstructure features at distinct length scales.

Multiscale analysis methods are a class of simulation methods that have become useful and important within the past decade[1-8]. Based on the process to integrate different computer models at various dimensions ranging from a fraction of a nanometer to meters into one computation scheme, the multiscale simulation could be divided into two categories, parallel and hieratical. Parallel multiscale simulation will

decompose the system into several domains, which simultaneously couple models of different scales and information is allowed to pass back and forth between different scales, e.g., concurrent hybrid model[2] and a monolithic effective scaling model[3, 4]. The atomistic simulation will be applied in the local region with serious deformation while the less expensive continuum method will be used for the far-field regions. For systems in which the scales are strongly coupled, it is necessary to consider scales in parallel. However, the handshaking interface between different scales could impose complicated problem and significant research effort has been dedicated to resolve the issue.

On the other hand, the hierarchical multiscale method treats the scales in a serial or sequential fashion, which is suitable for system that the scales are weakly coupled. Parameters are calculated from a small scale computational model and fed into model at a larger scale[5-8]. Hao *et al* [5] developed a two-level cell model (microcell and submicrocell) to consider two different impurity sizes, which is characteristic of such Fe-based alloys. The ductile fracture of a center cracked specimen is simulated using multi-scale hierarchical constitutive model for establishing the relationship between quantum mechanics, micromechanical and overall strength/toughness properties in steel design. Namilae and Chandra [6] employed molecular dynamics to simulate fiber pullout tests of carbon nanotubes(CNTs) in matrix, which are used to evaluate cohesive zone model parameters in finite element analysis to study the effect of interface strength on stiffness of the CNT-based composite. Houtte *et al* [7] proposed a multi-level model to study the plastic deformation of polycrystalline materials with texture-induced anisotropy. The parameters of a constitutive material model for finite element codes are identified for the simulation of metal forming processes. Although some multiscale models have been proposed, the development of hierarchical

simulation is still in its beginning stage. The proposed research will develop an hierarchical multiscale simulation approach that combine atomistic and continuum methods level by level to offer the possibility to link distinct length and implemented to carry out calculation of material properties that cannot be achieved otherwise.

The study on multiscale behavior will include various microstructures, i.e., grains and inclusion. In recent years, polycrystalline nanofilms have drawn increasing interest in both academia and industries. They have been proposed as the functional units for the construction of the future molecular-scale machines, and highly complex nanoelectromechanical systems (NEMS). Thin films are such important basic elements for advanced functional materials and devices that understanding their mechanical properties becomes more and more important. Significant research efforts have been made to investigate the size effects on the mechanical properties of nanofilms including theoretical, experimental methods and numerical simulations. Many experimental techniques have been developed to evaluate mechanical properties of nanofilms, including nanoindentation testing[9-11], x-ray diffraction with in situ tensile testing[12,13] and laser-ultrasonic surface acoustic wave spectrometry[14]. Some experiments[13,15-17] show the increase in elastic modulus as the constituent film size decreases while other experiments[9,12,14,18] show the opposite trend.

In addition to experimental characterization, the use of molecular simulations in the study of the mechanical properties of nanomaterials has given unique insight into the atomic scale phenomena including the processes that occur during plastic deformation. Some researchers studied the microstructure size effect on the plasticity behavior of materials. Yamakov *et al* [19-21] studied the nucleation of dislocations from the grain boundaries in nanocrystalline aluminum using molecular dynamics

simulation. However, most of the research focuses on single-crystalline or nanocrystalline materials since the simulated system sizes are limited to at most several hundred nanometers range. Since the grain size of polycrystalline nanofilms varies widely from 1μm to 10mm while the film thickness is in nanometer scale, it is impractical to employ solely molecular simulation to study the mechanical properties of the nanofilm due to the limitation of today's computers.

Impurities or inclusions are commonly observed inside metals. While some are added purposely to enhance the material strength, some appear inevitably due to the manufacturing process. The size of inclusion could vary from nanometers to micrometers, which would impose different effects on the material properties. Hence, a multiscale simulation is essential in order to properly address the impurity/inclusion size effect.

The proposed research is aimed to explore the effect of microstructures spanning several length scales to provide better understanding of the mechanisms that interconnect and interact to influence the mechanical properties. A multiscale method will be developed to bridge the gap between nanoscale and macroscale and study the multiscale behavior of materials. The proposed innovative algorithm adopts the representative volume element concept to link atomistic and continuum models through the device of the finite element method, which permits a reduction of the full set of atomistic degrees of freedom. This research gives a full description of the proposed innovative algorithm with special reference to the ways in which the method may be used to model crystals with more than a single grain or inclusion.

Approach

I. Innovative Hierarchical Multiscale Computation Method

Inspired by the concept of representative volume element (RVE) in dealing with heterogeneous materials, which consist of several materials or phases, the proposed multiscale simulation method will identify RVE of the system and study the properties of RVE from the individual constituent. It is clear that multiscale behavior and mechanical properties derived from bulk material are most likely erroneous for nano-scale materials. Their properties may vary locally over nanometer dimensions. Therefore, the determination of *in situ* mechanical behavior for nano-scale materials plays a crucial role for the development of nanoscience and a better understanding of nanoscale property can lead to unique nanostructures and innovative nanosystems for a wide range of applications including aerospace. In order to provide a correct description of nanomaterial properties, the constitutive relations for the single crystal will be examined thoroughly.

Molecular statics method will be adopted to study the deformation behavior of the RVE. Molecular statics simulations are implemented using conjugate gradient method, which carries out the energy minimization process in order to obtain the equilibrium atomic structure. The considered energy includes potential energy of interatomic interactions and potential energy due to external loading. Without loss of generality, face-center-cubic copper is chosen for this study. Embedded-atom-method (EAM) potential first developed by Foiles, Baskes, and Daw [22] is chosen to describe atomic interactions. In EAM potential, the total energy is composed of the electrostatic pairwise interaction energy between atoms and the embedding energy required to insert the atom into the local electron density field created by its near neighbors.

First, the constitutive relation of the single crystalline nanofilm is investigated thoroughly. The periodic boundary condition (PBC) is applied in both inplane

direction to simulate an infinite large film. Minimum image criterion is adopted to implement the periodic boundary condition. Uniaxial strain deformation is loaded on nanofilms to extract their elastic and plastic properties. In continuum mechanics, once the elastic properties along one set of coordinate system is known, the material properties along any rotated coordinate system could be calculated through coordinate transformation method. However, it is not clear whether the coordinate transformation relationship could be applied to predict the film thickness dependent elastic properties along any crystallographic orientation. Besides, the applicability of single crystal plasticity, which has been well developed, on the single crystalline nanafilm will also be examined. Hence, the size dependent elastic and plastic properties along different crystal orientations will be examined and compared with the prediction made by coordinate transformation method and single crystal plasticity.

Once the mechanical properties of single crystalline nanofilm along any crystal orientation could be realized effectively, the material information will be employed in finite element model as parameters to study the macro-mechanical deformation of the large system. We are going to utilize the developed hierarchical multiscale method to study the grain and inclusion effect.

II. Polycrystalline Nanofilm

In the proposed research, the size dependence of mechanical properties for polycrystalline nanofilm, which contains grains with different crystal orientation, will be investigated. Metallic polycrystalline nanofilms, grown by almost any deposition method onto amorphous substrates, show at least some degree of crystallographic texture[23], which induces macroscopic anisotropy. The observed texture mostly displays a fiber texture, in which the surface normal of the grains are nearly parallel to

a specific crystallographic direction while a random orientation of grains is simultaneously maintained in the plane of the film. With the recent advance of nanotechnology, it provides a unique opportunity to have an in-depth understanding of how the mechanical properties of polycrystalline nanofilms depend on the characteristic size of microstructure and the film thickness.

The polycrystalline film is assumed to be composed of the hexagonal grains with size on the order of micrometers. The arrangements of the grain crystallographic orientations are random with out-of-plane normal direction fixed at certain crystallographic direction. The principal in-plane directions of each grain are randomly distributed. Each individual grain is still a coarse grain of at least micron size. Each hexagonal grain is constructed by rotating the original film with in-plane directions by a random angle varied from 0 to $\pi/2$ due to the crystallographic symmetry.

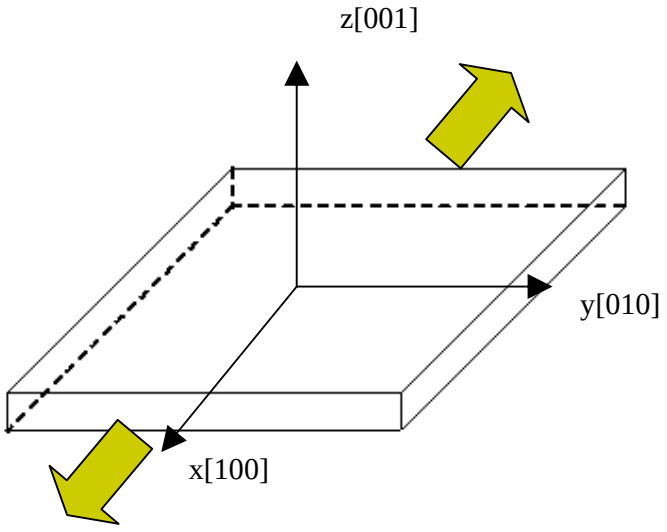
A macroscale representative material point in each grain of the nanofilm can be regarded as an infinite large single crystalline nanofilm composed of discrete atoms due to the huge difference in two characteristic sizes, i.e., grain size and film thickness. Each grain could be regarded as a RVE. Since the crystal orientation of each grain is different, the constitutive relation in terms of global coordinate would be quite different. With such large size scale, it is impractical to employ the molecular simulation solely to analyze the grain effect. For polycrystalline nanofilm, the scales of grain size and film thickness are weakly coupled. Hence, hierarchical multiscale method is a reasonable choice for the study on the size dependence of mechanical properties. The material properties of RVE can be obtained for the material point through analyzing the atomic structure underlying the material point. The constitutive relations derived in this manner are able to capture the nanosize effect and include it

in the continuum model at macro/micro-scale.

Results and Discussion

The proposed research developed a hierarchical multi-scale simulation method that is computationally more efficient and can better reflect the multiscale material reality as compared to conventional approaches such as molecular dynamics.

The constitutive relations of the single crystalline nanofilm along different crystal orientations as shown in Figure 1 are investigated thoroughly under simple tension test. It is noticed that the out-of-plane crystal orientation is fixed at [001] direction. The film thickness dependences of elastic properties for nanofilms with different in-plane crystal orientations are shown in Figure 2 and 3. It is noticed that the size dependence of Young's modulus would be significantly affected by the crystal orientation. The applicability of coordinate transformation relation would be examined through the prediction of the size dependent elastic properties along different crystal orientation.



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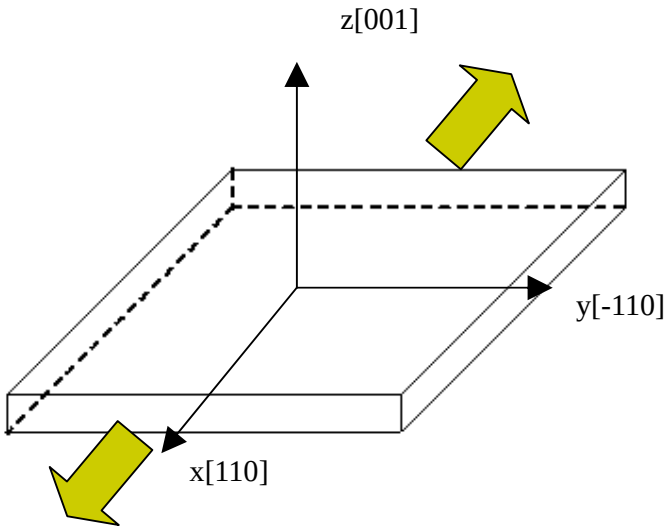

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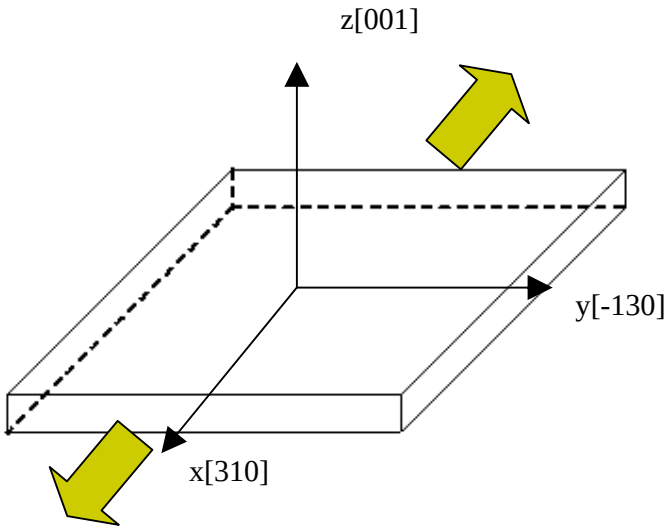
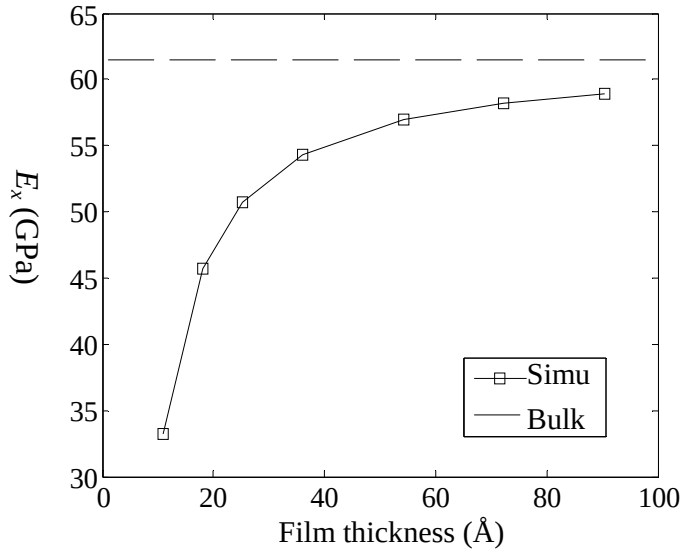


Figure 1. The crystal orientation of single crystalline nanofilm under simple tension test. (a) x[100], y[010], z[001], (b) x[110], y[-110], z[001], and (c) x[310], y[-130], z[001]



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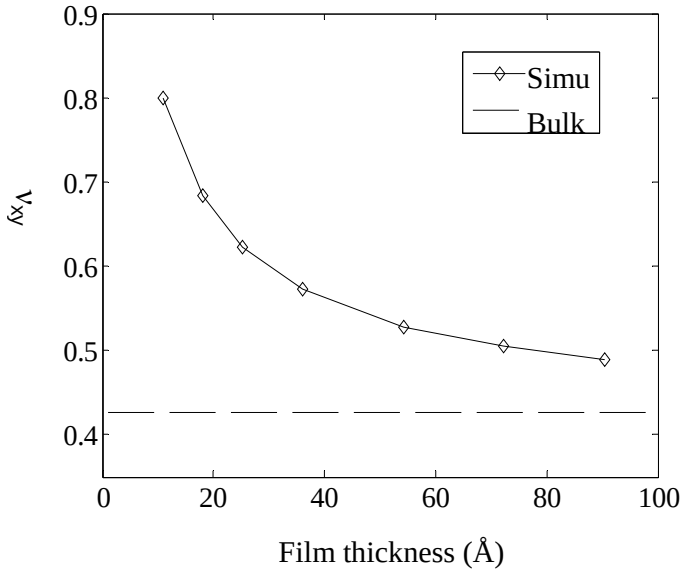

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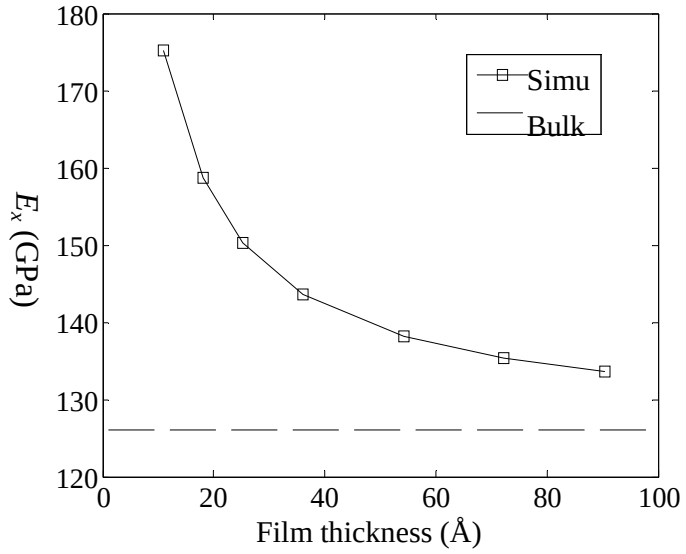
Figure 2. The size dependences of Young's modulus and Poisson's ratio for single crystalline nanofilms with crystal orientation of x[100], y[010], z[001].



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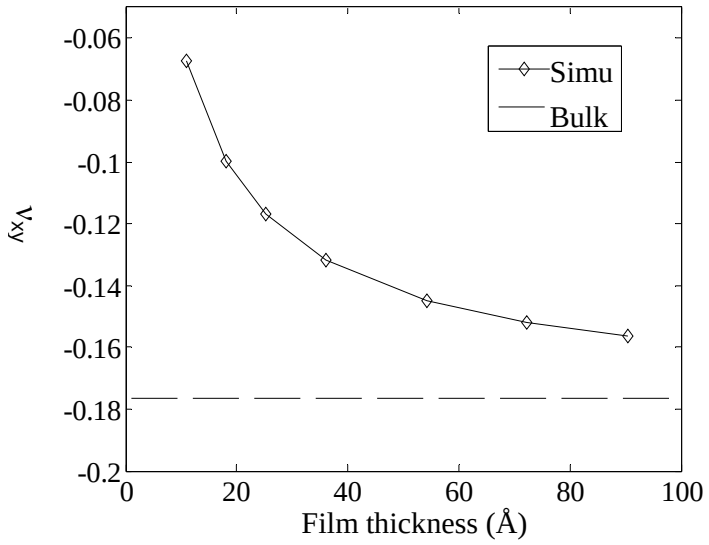


(b)

Figure 3. The size dependences of Young's modulus and Poisson's ratio for single crystalline nanofilms with crystal orientation of x[110], y[-110], z[001].

In continuum mechanics, if the elastic properties at one coordinate system are known, the elastic properties along rotated coordinate system could easily be obtained

from the coordinate transformation relation. Suppose the general compliance matrix could be expressed as

$$[S]=\begin{bmatrix} \frac{1}{E_x} & -\frac{\nu_{yx}}{E_y} & -\frac{\nu_{zx}}{E_z} & \frac{\eta_{yz,x}}{G_{yz}} & \frac{\eta_{xz,x}}{G_{xz}} & \frac{\eta_{xy,x}}{G_{xy}} \\ -\frac{\nu_{xy}}{E_x} & \frac{1}{E_y} & -\frac{\nu_{zy}}{E_z} & \frac{\eta_{yz,y}}{G_{yz}} & \frac{\eta_{xz,y}}{G_{xz}} & \frac{\eta_{xy,y}}{G_{xy}} \\ -\frac{\nu_{xz}}{E_x} & -\frac{\nu_{yz}}{E_y} & \frac{1}{E_z} & \frac{\eta_{yz,z}}{G_{yz}} & \frac{\eta_{xz,z}}{G_{xz}} & \frac{\eta_{xy,z}}{G_{xy}} \\ \frac{\eta_{x,yz}}{E_x} & \frac{\eta_{y,yz}}{E_y} & \frac{\eta_{x,yz}}{E_z} & \frac{1}{G_{yz}} & \frac{\mu_{xz,yz}}{G_{xz}} & \frac{\mu_{xy,yz}}{G_{xy}} \\ \frac{\eta_{x,xz}}{E_x} & \frac{\eta_{y,xz}}{E_y} & \frac{\eta_{z,xz}}{E_z} & \frac{\mu_{yz,xz}}{G_{yz}} & \frac{1}{G_{xz}} & \frac{\mu_{xy,xz}}{G_{xy}} \\ \frac{\eta_{x,xy}}{E_x} & \frac{\eta_{y,xy}}{E_y} & \frac{\eta_{z,xy}}{E_z} & \frac{\mu_{yz,xy}}{G_{yz}} & \frac{\mu_{xz,xy}}{G_{xz}} & \frac{1}{G_{xy}} \end{bmatrix},$$

the compliance matrix at the rotated coordinate system could be obtained from

$S'_{mnop}=\beta_{mi}\beta_{nj}\beta_{ok}\beta_{pl}S_{ijkl}$, where $\beta_{ij}=\hat{e}'_i\bullet\hat{e}_j$. For single crystalline nanofilm, the compliance matrix could be simplified as

$$[S]=\begin{bmatrix} \frac{1}{E_x} & -\frac{\nu_{xy}}{E_x} & 0 \\ -\frac{\nu_{xy}}{E_x} & \frac{1}{E_x} & 0 \\ 0 & 0 & \frac{1}{G_{xy}} \end{bmatrix}.$$

The elastic constants of nanofilm at the rotated coordinate system could be written as

$$\frac{1}{E'_x}=\frac{1}{E_x}\cos^4\theta+\left(\frac{1}{G_{xy}}-\frac{2\nu_{xy}}{E_x}\right)\sin^2\theta\cos^2\theta+\frac{1}{E_x}\sin^4\theta$$

$$\nu'_{xy}=E'_x\left[\frac{\nu_{xy}}{E_x}-\left(\frac{2}{E_x}+\frac{2\nu_{xy}}{E_x}-\frac{1}{G_{xy}}\right)\sin^2\theta\cos^2\theta\right]$$

$$\frac{1}{G'_{xy}}=\frac{1}{G_{xy}}+4\left(\frac{2}{E_x}+\frac{2\nu_{xy}}{E_x}-\frac{1}{G_{xy}}\right)\sin^2\theta\cos^2\theta$$

$$\frac{\eta'_{xy,y}}{G'_{xy}} = \frac{\eta'_{y,xy}}{E'_x} = \left(\frac{2\nu_{xy}}{E_x} + \frac{2}{E_x} - \frac{1}{G_{xy}}\right)\cos^3\theta\sin\theta + \left(-\frac{2\nu_{xy}}{E_x} - \frac{2}{E_x} + \frac{1}{G_{xy}}\right)\cos\theta\sin^3\theta$$

$$\frac{\eta'_{xy,x}}{G'_{xy}} = \frac{\eta'_{x,xy}}{E'_x} = \left(-\frac{2\nu_{xy}}{E_x} - \frac{2}{E_x} + \frac{1}{G_{xy}}\right)\cos^3\theta\sin\theta + \left(\frac{2\nu_{xy}}{E_x} + \frac{2}{E_x} - \frac{1}{G_{xy}}\right)\cos\theta\sin^3\theta$$

where θ is the angle between the rotated x' direction and the original x direction. However, the shear modulus is not easy to obtain from current simulation setup since the periodic boundary box is set to be rectangular. The size dependent shear modulus could be calculated from the elastic constants of nanofilms along x[100], y[010], z[001], and x[110], y[-110], z[001] as

$$\frac{1}{E[110]} = \frac{1}{E_x}\cos^4\frac{\pi}{4} + \left(\frac{1}{G_{xy}} - \frac{2\nu_{xy}}{E_x}\right)\sin^2\frac{\pi}{4}\cos^2\frac{\pi}{4} + \frac{1}{E_x}\sin^4\frac{\pi}{4}.$$

Figure 4 shows the calculated size dependent shear modulus for crystal orientation x[100], y[010], z[001] nanofilm. It is observed as the film get thicker, the shear modulus would decrease and approach the bulk value.

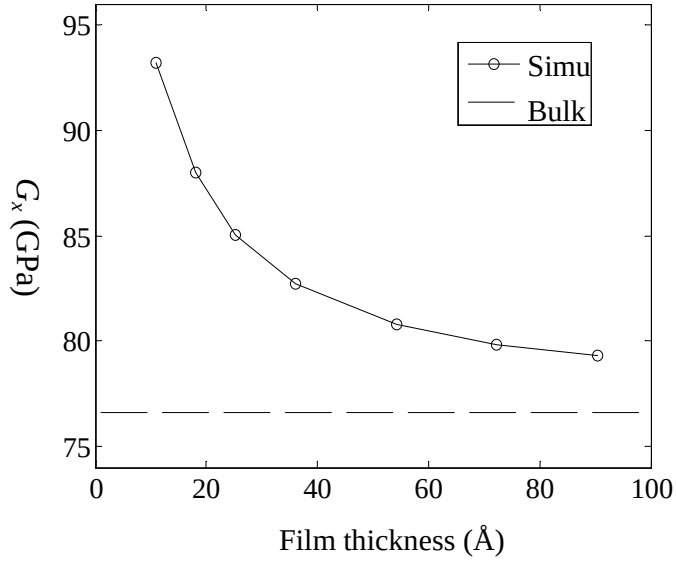
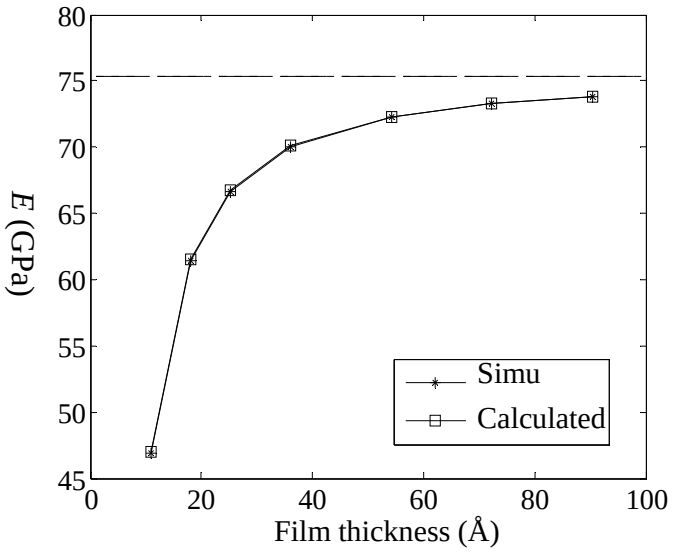


Figure 4. The size dependences of shear modulus calculated for single crystalline

nanofilms with crystal orientation of x[100], y[010], z[001].

Hence, the elastic constants of nanofilms along x[310], y[-130], z[001] crystal orientation could be predicted based on coordinate transformation relation and compared with the simulated results as depicted in Figure 5. It is noted that the calculated values and the simulation results agree quite well, which indicate that the coordinate transformation relation of elastic properties could still apply to single crystalline nanofilm with fixed out-of-plane crystal orientation.



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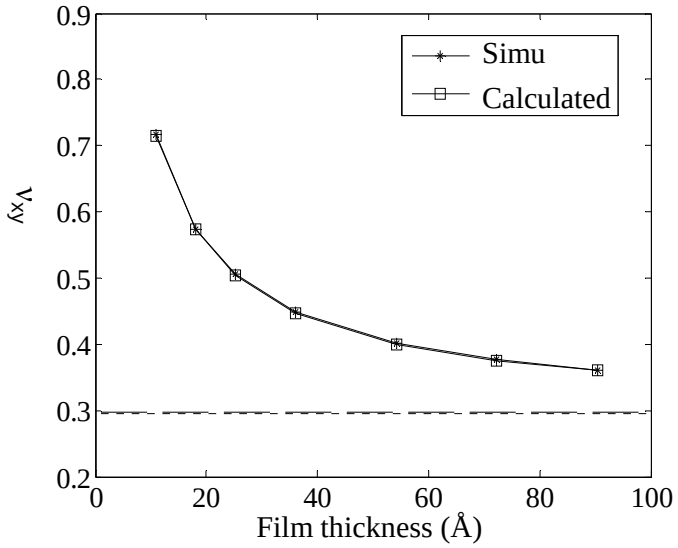

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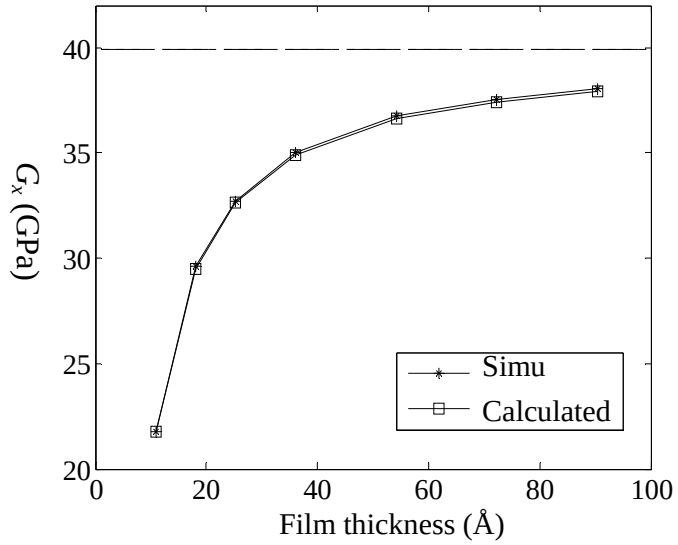


(c)

Figure 5. The comparison between the predicted elastic constant of nanofilms based on coordinate transformation relation and the molecular simulation results. (a) Young's modulus, (b) Poisson's ratio and (c) shear modulus

The textured polycrstalline nanofilm is assumed to be composed of the hexagonal grains with size, *d*, on the order of micro-meters. The arrangements of the grain crystallographic orientations are random with out-of-plane normal direction fixed at the [001] direction. Each hexagonal grain is constructed by rotating the original film with in-plane directions (x [100] and y [010]) by a random angle, θ, as shown in Figure 6. The rotating angle varies from 0 to $\pi/2$ due to the crystallographic symmetry.

Since the grain size is in the micro-meter range while the film is in nanometer range, each grain could be treated as single crystalline nanofilms whose elastic properties could be obtained from coordinate transformation relation. In order to examine the grain size effect, models with four different grain sizes (2.5, 6.25, 12.5 and 25 μ m) are constructed. Since the grain orientations are random, each grain size model is simulated five times with different grain orientations to attain the statistical significance. Also, two different model size, L (75 and 300 μ m), are built to check the convergence of the results. Plane stress condition is assumed for the film. The finite element mesh for the polycrystalline nanofilm is shown in Figure 7.

In order to obtain the elastic constants of the textured polycrystalline nanofilm, a small deformation is applied along one direction with all three other in-plane sides are fixed as shown in Figure 6. The effective strains and stress on the polycrystalline nanofilm could be attained as

$$\bar{\varepsilon}_{XX} = \frac{u_x}{L}, \quad \bar{\varepsilon}_{YY} = 0$$

$$\bar{\sigma}_{XX} = \frac{F_X}{Lt}, \quad \bar{\sigma}_{YY} = \frac{F_Y}{Lt}$$

where F_X and F_Y are reaction forces at the fixed boundary due the applied displacement and t is the film thickness. If the grain orientations are random enough and the finite element model includes enough grains, the elastic properties along X and Y directions should be equivalent. Since plane stress condition along film thickness is assumed ($\overline{\sigma_{ZZ}} = 0$), the effective stress-strain relation could be written as

$$\bar{\varepsilon}_{XX} = \frac{1}{\bar{E}}(\bar{\sigma}_{XX} - \bar{\nu}\bar{\sigma}_{YY})$$

$$\bar{\varepsilon}_{YY} = \frac{1}{\bar{E}}(\bar{\sigma}_{YY} - \bar{\nu}\bar{\sigma}_{XX}) .$$

Therefore the effective in-plane Young's modulus and Poisson's ratio could be calculated as shown in Figure 8 and 9. It is notice that if the small model size is adopted for the analysis, it could easily draw the wrong conclusion that the grain size would affect the effective elastic constants of texture polycrystalline nanofilm. From the results using larger model, we observe the effective elastic constants would not be influenced by the grain size even though the data for the same grain size deviates.

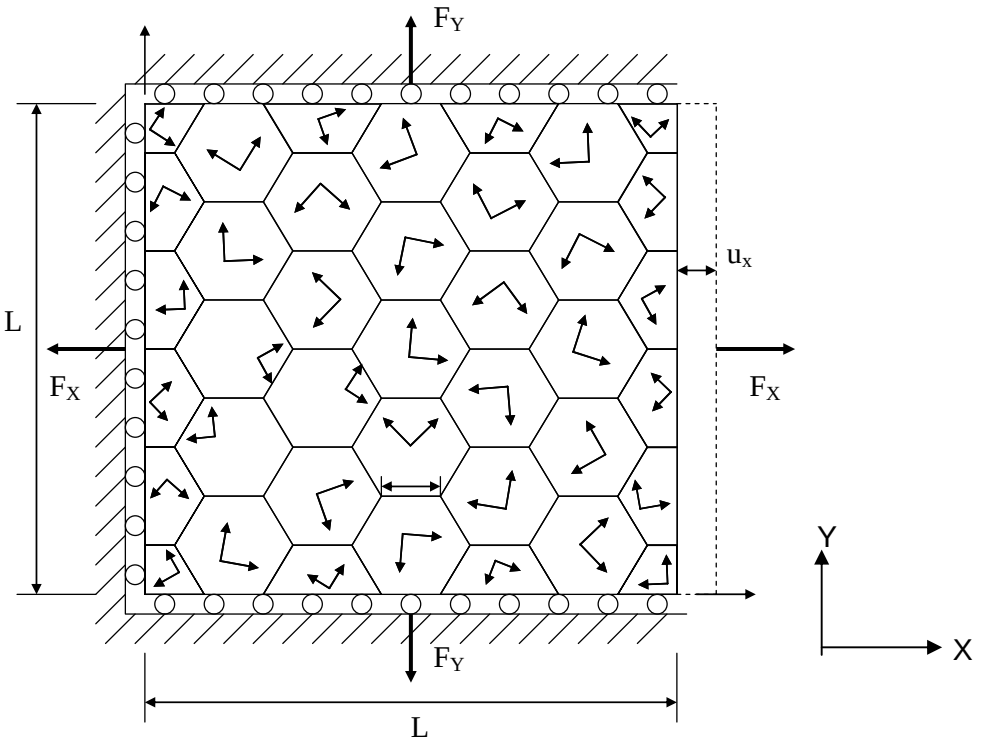


Figure 6. The schematic configuration of textured polycrystalline nanofilm.

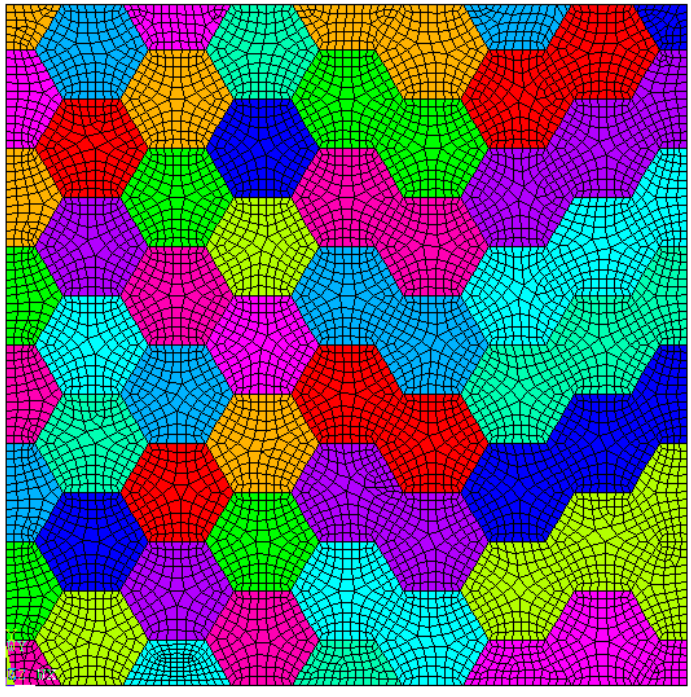
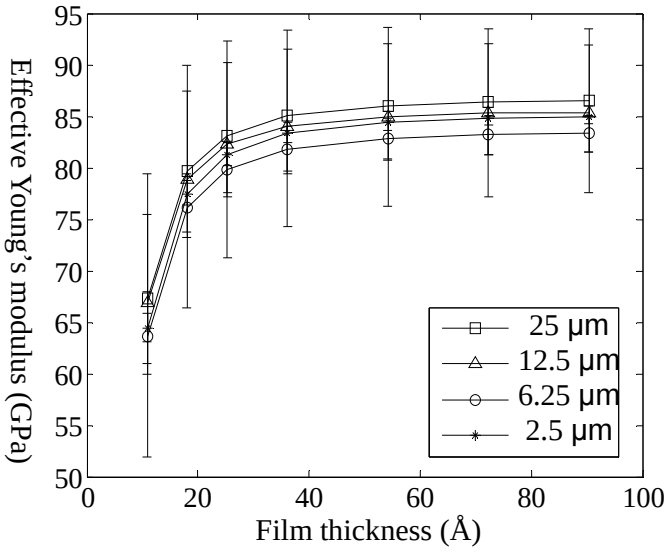
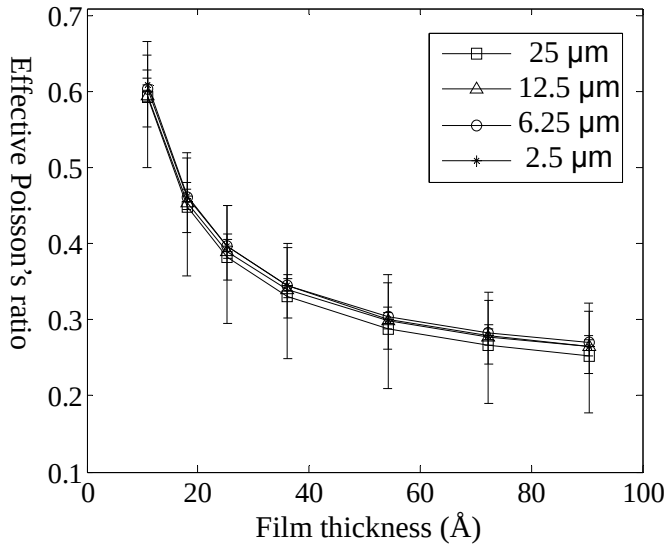


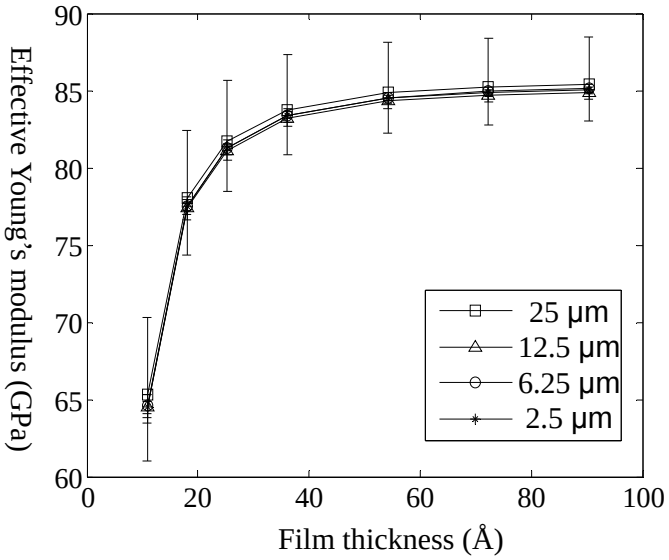
Figure 7. The finite element mesh for the polycrystalline nanofilm.



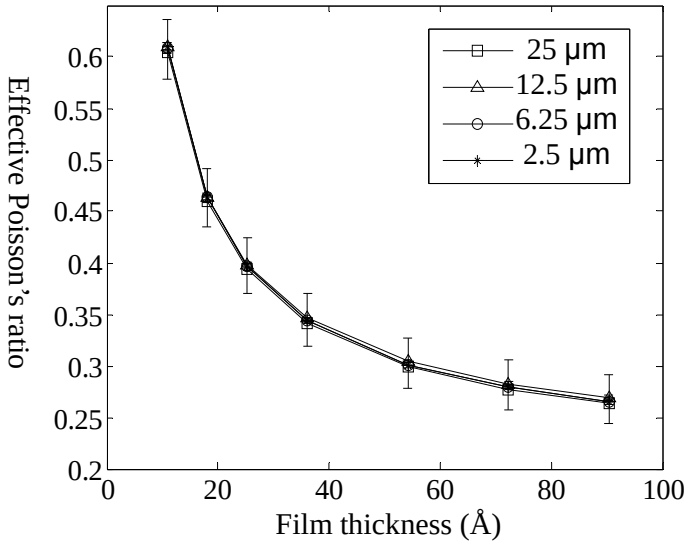


(b)

Figure 8. The effective elastic properties of textured polycrystalline nanofilm simulated with 75 μ m model size.



(a)



(b)

Figure 9. The effective elastic properties of textured polycrystalline nanofilm simulated with 300 μ m model size.

Conclusion

The proposed project is meant for the development of a hierarchical multiscale simulation method for the quantification of the microstructure effect on material properties with characteristic features spanning several length scales. A computational approach based on the concept of representative volume element in dealing with heterogeneous materials, which consist of several materials or phases, was developed. The proposed approach that links atomistic and continuum models sequentially was employed to quantify the grain size and film thickness effect on mechanical properties of textured polycrystalline nanofilms. The multiscale analysis for system-level prediction could be realized since the grain size is in micrometers and the film thickness is in nanometers. If combined with the experimental study, a systematic method will be established to characterize the microstructure effect. The method will constitute a breakthrough in charactering size dependent material properties and benefit innovative fabrication processes and unique design of nano-scale devices. Moreover with the proper identification of representative element and full understanding of its properties, the microstructure effect on macroscopic material properties could be realized easily with affordable computational effort.

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